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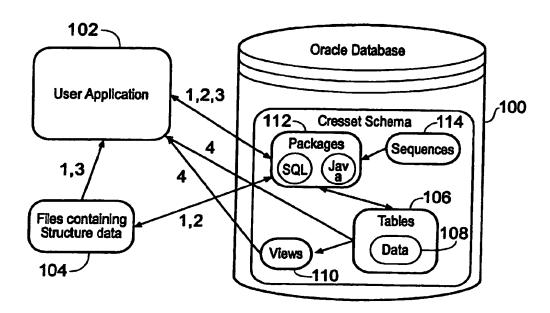
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(54) Title: SEARCHABLE MOLECULAR DATABASE



(57) Abstract: A computer system comprising a database (100) having a plurality of records is provided. Each record comprises a filed point representation representing field extrema for a conformation of a chemical structure. The database may include records for multiple conformations of the same chemical structure. Each record can have a searchable index of the filed point representation. In one embodiment the index is bit string. An indexing mechanism for generating an index, a searching mechanism for searching the database and a graphical user interface to enable a user to interface with the database (100) are also provided.

# WO 2004/023337 A1



Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

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A. CLASSIFICATION OF SUBJECT MATTER IPC 7 G06F17/30 G06F17/50

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According to International Patent Classification (IPC) or to both national classification and IPC

#### B. FIELDS SEARCHED

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Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the International search (name of data base and, where practical, search terms used)

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*A* document cons  *E* earlier filing  *L* document which citati  *O* document other  *P* document later  Date of the	categories of cited documents:  ment defining the general state of the art which is not lidered to be of particular relevance of document but published on or after the international date ent which may throw doubts on priority claim(s) or his cited to establish the publication date of another on or other special reason (as specified) ment referring to an oral disclosure, use, exhibition or means ment published prior to the international filing date but than the priority date claimed	'T' later document published after the interpretation or priority date and not in conflict with cited to understand the principle or the invention  'X' document of particular relevance; the cannot be considered novel or cannot involve an inventive step when the decannot be considered to involve an indocument is combined with one or ments, such combination being obvious the art.  '&' document member of the same patent	emational filing date the application but eory underlying the claimed invention t be considered to ocument is taken alone claimed invention iventive step when the ore other such docu- us to a person skilled family

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